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Two Methods for Modelling the Propagation of Terahertz Radiation in a Layered Structure

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Abstract. Modelling the interaction of terahertz (THz) radiation with biological tissue poses many interesting problems. THz radiation is neither obviously described by an electric field distribution or an ensemble of photons and biological tissue is an inhomogeneous medium with an electronic permittivity that is both spatially and frequency dependent making it a complex system to model.

A three-layer system of parallel-sided slabs has been used as the system through which the passage of THz radiation has been simulated. Two modelling approaches have been developed a thin film matrix model and a Monte Carlo model. The source data for each of these methods, taken at the same time as the data recorded to experimentally verify them, was a THz spectrum that had passed though air only.

Experimental verification of these two models was carried out using a three-layered *in vitro* phantom. Simulated transmission spectrum data was compared to experimental transmission spectrum data first to determine and then to compare the accuracy of the two methods. Good agreement was found, with typical results having a correlation coefficient of 0.90 for the thin film matrix model and 0.78 for the Monte Carlo model over the full THz spectrum. Further work is underway to improve the models above 1 THz.

Key words: Biological tissue, modelling, Monte Carlo, simulation, skin, terahertz

1. Introduction

Following developments in THz generation and detection THz radiation has become a point of interest regarding its use in a medical physics environment. The mechanisms of interaction of THz radiation with tissue [1] suggest that it could have applications in the study of biological tissues. Understanding the mechanism for the interaction of THz radiation with biological tissue is essential for developing the possible medical applications of THz radiation.

Specific molecular and DNA resonances occur at THz frequencies and have been investigated in previous studies. Diatomic molecules have consecutive rotational states, which are separated in energy terms by a gap corresponding to a THz frequency. Similarly amino acids, peptides and proteins have molecular rotation and vibrational modes that are separated by energies that correspond to THz frequencies, as does DNA. THz radiation, it has been suggested may also interact with cellular structure itself, in particular regions of the cell with increased index of refraction, for example the membrane or the cellular organelles. In much of this research the particular molecule or cellular unit has been isolated before irradiation. However with *in vivo* measurements, though these molecules are present, the particular modes of vibration may be constricted by the structure of the tissue around them or more likely overshadowed by a more dominant interaction, namely the absorption of THz radiation by water.

THz radiation is readily absorbed by water and as such has a low penetration depth in biological tissue, at most a few millimetres within fatty tissue [2]. Hence THz radiation is being investigated as a diagnostic tool for diseases of human surface tissue the most accessible of which is skin. Studies have shown that THz radiation is able to distinguish between the stratum corneum, epidermis and dermis in reflection images of skin taken using a terahertz pulsed imaging (TPI) system [3].

A tool developed to simulate the passage of THz radiation though a skin like system would be of use to future clinical trials investigating possible techniques for the use of THz radiation in the detection or diagnosis of skin diseases. The structure of skin is commonly modelled as a series of parallel-sided slabs, [4, 5] the use of three layers replicates the stratum corneum, epidermis and dermis, the features of human skin resolved by THz pulsed reflection imaging [3]. Each of these layers will have their own dimension and frequency dependent physical properties.

Two models were developed to simulate this three layered system, a thin film matrix model and a Monte Carlo model. A simplified *in vitro* phantom was constructed using two layers of TPX (poly-4-methylpent-1-ene), a material with constant physical properties in the THz frequency range, encasing a water based solution with frequency dependent physical properties.

2. Experimental Method

The phantom was constructed of two 2 mm layers of TPX encasing a 180 μm layer of water/propanol-1 solution. In order to ensure a clear signal through the cell the water was mixed with propanol-1 a material with a much lower absorption coefficient than water in the THz frequency range. Thirteen water/propanol-1 concentrations, from 50% water/propanol-1 to 100% propanol-1 were used. The experimental layout can be seen in Figure 1, the THz radiation was incident normally upon the sample. Point measurements of the transmitted pulse were recorded.

TPX has an index of refraction of 1.43 [6]. The Leeds TPI system has a THz frequency content up to 3.5 THz, measurements have shown negligible absorption within this frequency range and an approximation was made that the absorption of the TPX layer was zero in this frequency range.

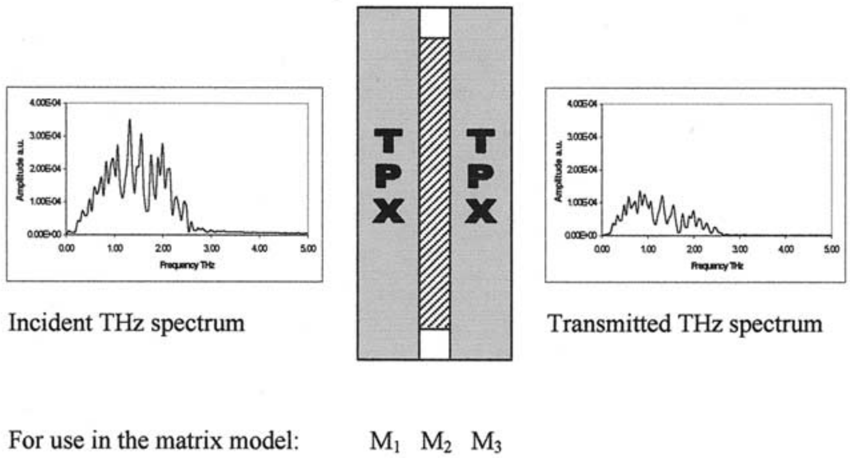

Figure 1. Schematic diagram of the three-layer phantom, the shaded area represents the water/propanol-1 solution.

The refractive index of water and propanol-1 were determined using the Cole-Cole model. (1) The Cole-Cole model is a way of describing the complex permittivity of a given polar solution as a function of frequency. The numerical parameters used in the Cole-Cole model were taken from Kindt et al. [7] and have been validated up to 1 THz.

$$\varepsilon(\omega) = \varepsilon_\infty + \sum_{j=1}^{n} \frac{\varepsilon_j - \varepsilon_{j+1}}{\left[1 + (i\omega\tau_j)^{1-\alpha_j}\right]^{\beta_j}} \tag{1}$$

As

$$\varepsilon(\omega) = (n(\omega) + ik(\omega))^2$$

Where $k(\omega) = \lambda\alpha(\omega)/4\pi$ where λ is the wavelength of the incident radiation and $\alpha(\omega)$ is the absorption coefficient of the sample medium. Real and imaginary parts of this expression can be equated to solve for the index of refraction and absorption coefficient. These were then averaged, using volume weighting, to determine the appropriate values for of the thirteen water/propanol-1 solutions.

3. The Thin Film Matrix Model

The thin film model simulates mathematically the change in the incident electric field as it passes through the medium. The change in amplitude was calculated for each frequency point in the spectrum using the appropriate electric permittivity value for the specific frequency under consideration. Each layer of material is described mathematically by a matrix of the form.

$$M_i = \begin{pmatrix} \cos\left(\frac{2\pi}{\lambda} h_i(a_i + ib_i)\right) & \frac{i}{a_i + ib_1}\sin\left(\frac{2\pi}{\lambda} h_i(a_i + ib_i)\right) \\ i(a_i + ib_i)\sin\left(\frac{2\pi}{\lambda} h_i(a_i + ib_i)\right) & \cos\left(\frac{2\pi}{\lambda} h_i(a_i + ib_i)\right) \end{pmatrix}$$

Where $n_i = a_i + ib_i$ the complex index of refraction and h_i is the thickness of a given layer i, and λ is the wavelength of the incident radiation.

Multiplying the three appropriate matrices together, as shown in Figure 1, gives:

$$M = M_3 M_2 M_1 = \begin{pmatrix} m_{11} & im_{12} \\ im_{21} & m_{22} \end{pmatrix}$$

Where the ratio of the transmitted amplitude to the incident amplitude T was given by:

$$T = \frac{2}{m_{11} + m_{22} + i(m_{12} + m_{21})}$$

And the ratio of the reflected amplitude to the incident amplitude was given by:

$$R = \frac{(m_{11} - m_{22}) + i(m_{12} - m_{21})}{(m_{11} + m_{22}) + i(m_{12} + m_{21})}$$

4. The Monte Carlo Model

The THz spectrum was converted into a photon distribution, using a statistical sampling technique. As the THz beam incident on the sample is also coherent the technique also incorporated modulation by a Poisson distribution.

The Monte Carlo code tracked the position of the photon though the sample, determining its position and probability of interaction at any particular position in the sample. The Fresnel coefficients determined the probability passing through a junction between two layers. In the TPX the photon continued, travelling in the same direction until it reached a TPX/air or TPX/water/propanol-1 boundary. In the water/propanol-1 solution an absorption interaction was included by sampling a Beer-Lambert probability distribution after each mean free path to determine whether the photon in question should continue on its flight or if an absorption event should occur within the simulation.

In this way the number of photons exiting the sample could be counted, both the transmitted and reflected spectra.

5. The Graphical Comparison

Comparing experimental and simulated results using the thin layer model was trivial as the data was expressed in the same units. However, as the simulated Monte

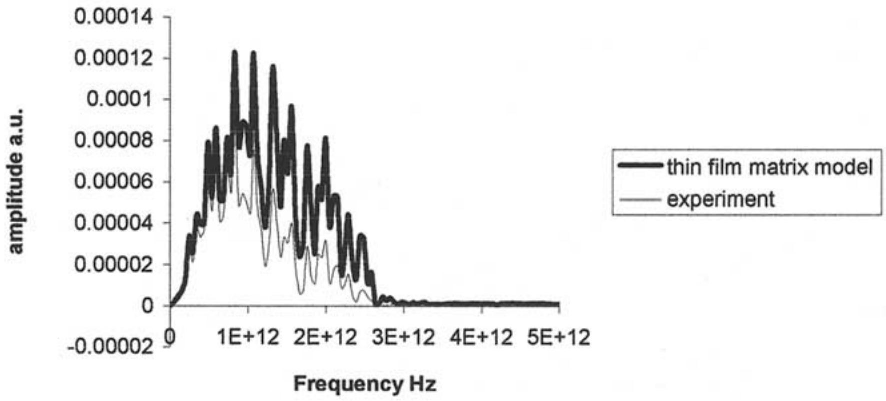

Figure 2a. A graph showing the comparison of the experimental results and the spectrum simulated using the thin film matrix model, over the whole frequency range for a water/propanol-1 solution with 54% propanol-1.

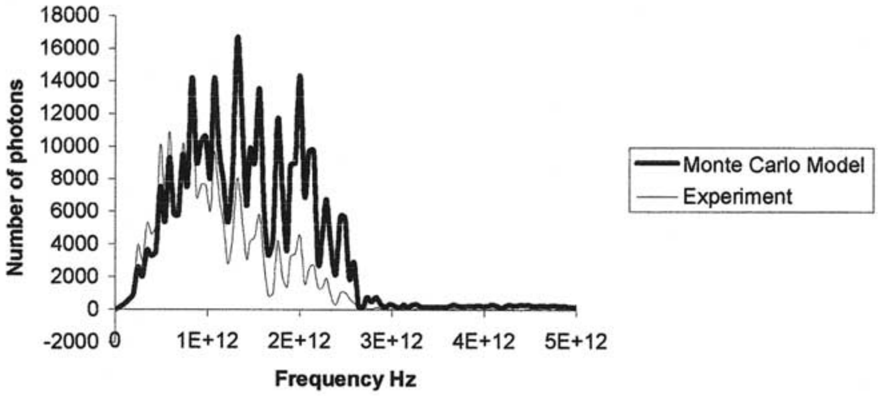

Figure 2b. A graph showing the comparison of the experimental results and the spectrum simulated using the Monte Carlo model, over the whole frequency range for a water/propanol-1 solution with 54% propanol-1.

Carlo results were expressed as the number of photons at a specific frequency, the corresponding experimental result was converted into a photon distribution using the sampling procedure described above.

6. Results

Comparisons of the simulations with the experimental results for a water/propanol-1 solution with 54% propanol-1 solutions are shown in Figures 2 and 3.

The amplitudes of the simulated and experimental spectra were compared using regression analysis. If the two coincided completely then any best-fit line would correspond to the identity, y=x. Looking at the best-fit line of the form y = bx +a and

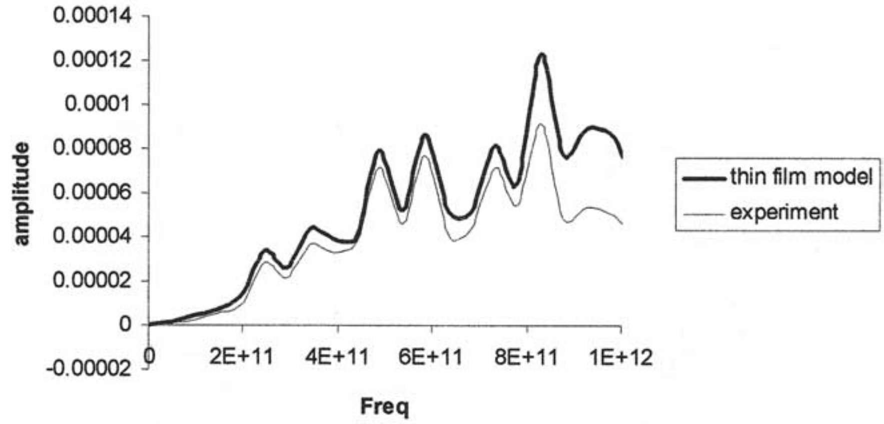

Figure 3a. A graph showing the comparison of the experimental results and the spectrum simulated using the thin film matrix model up to 1 THz for a water/propanol-1 solution with 54% propanol-1.

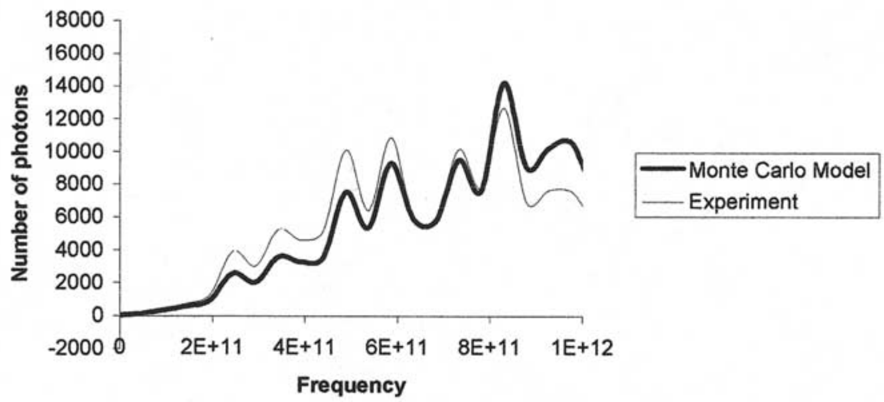

Figure 3b. A graph showing the comparison of the experimental results and the spectrum simulated using the Monte Carlo model up to 1 THz for a water/propanol-1 solution with 54% propanol-1.

calculating the correlation coefficient, r^2, of this fit enables first an assessment of experimental and simulation correlation. It also gives a way of comparing each simulation as it is independent of the amplitude scale. For solutions of water/propanol-1 with 54% propanol-1 the regression coefficients are shown in Table I, both for the full spectrum and up to 1 THz.

Table I. Table I shows the correlation coefficient r^2 and the parameters of the regression line y=bx+a that has been fitted to the plot of the amplitude of the simulated and experimental data, for a propanol-1 concentration of 54%. Data is given, in both the thin film matrix model and the Monte Carlo model, over the full THz spectrum and up to 1 THz.

Propanol-1 Concentration	Thin film matrix model			Monte Carlo Model		
% by volume	r^2	b	a	r^2	b	a
Full spectrum 54	0.90	0.59	–5.59e-8	0.78	0.59	8.11
Up to 1 THz 54	0.92	0.73	2.45e-6	0.86	0.83	1039.26

7. Conclusions

Both the thin film and Monte Carlo results simulate the overall trend and smaller details of the experimental THz spectrum. Up to 1 THz there was also a good match between simulated and experimental amplitudes. At higher frequencies both models fail to simulate the amplitude of the experimental spectrum. The thin film analysis provides in general a better amplitude match than the Monte Carlo simulation over the whole frequency spectrum. Both succeed at this task below 1 THz as can also be seen in Figures 2 and 3. The Monte Carlo model tended to underestimate the magnitude of the experimental amplitude at lower frequencies and then over estimate it increasingly as the frequency increased. The thin film model increasingly overestimated as the frequency increased.

Further work is underway to determine the effect or variation in the values of the optical parameters. The general trend to the increasing inaccuracy of the models to simulate the amplitude seen in the experimental case suggests an underestimation of absorption coefficient of the water/propanol-1 solution. The Cole-Cole model has only been validated with the parameters used up to 1 THz. It could be that the Cole-Cole model is an inappropriate distribution for the response of a polar liquid irradiated with higher frequency radiation, or it could be that the parameters used within the Cole-Cole model are incorrect to describe the effect of THz radiation on a polar liquid.

The success of the two models up to 1 THz, were the optical parameters have been experimentally validated, has encouraged the extension of the models to simulated the passage of THz radiation through skin. In this case each of the three layers described will have a complex spatially dependent electric permittivity and each will have unique dimensions. Measurements on human skin are to be made *in vitro* and *in vivo* in reflection and transmission modes to further test the models.

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